POVMs: a small but important step beyond standard quantum mechanics

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It is the purpose of the present contribution to demonstrate that the generalization of the concept of a quantum mechanical observable from the Hermitian operator of standard quantum mechanics to a positive operator-valued measure is not a peripheral issue, allegedly to be understood in terms of a trivial nonideality of practical measurement procedures, but that this generalization touches the very core of quantum mechanics, viz. complementarity and violation of the Bell inequalities.

Keywords: Positive operator-valued measure; complementarity; Bell inequalities.

1. Introduction

I shall refer to the usual quantum mechanical formalism dealt with in quantum mechanics textbooks as the *standard* formalism. In this formalism a quantum mechanical (standard) observable is represented by a Hermitian operator, having a spectral representation consisting of projection operators E_m, which constitute an *orthogonal* ($TrE_mE_{m'} = O,\ m \neq m'$) decomposition of the identity operator,

$$E_m \geq O,\ E_m^2 = E_m,\ \sum_m E_m = I.$$

The projection operators E_m are said to generate a projection-valued measure (PVM). A *generalized* observable is represented by a positive operator-valued measure (POVM), generated by a set of non-negative operators M_m that in general are *not* projection operators and constitute a *non*-orthogonal decomposition of the identity operator, i. e., in general $TrM_mM_{m'} \neq O$, and

$$M_m \geq O,\ \sum_m M_m = I. \tag{1}$$

In generalized quantum mechanics measurement probabilities are given according to

$$p_m = Tr\rho M_m, \tag{2}$$

ρ a density operator, and the set $\{M_m\}$ satisfying (1). In the following generalized and standard observables will be referred to by their POVM and PVM, respectively.

Nowadays it is more and more realized that standard quantum mechanics is not completely adequate for dealing with quantum information, and that it is necessary to consider POVMs. Thus, as is well known, standard observables can only yield information on *diagonal* elements of ρ. Since in general the operators M_m of a POVM need not commute with each other, POVMs may yield information on *off-diagonal* elements of ρ, too. Particularly interesting is the existence of *complete* POVMs allowing to reconstruct the density operator from the set of probabilities (2) obtained in a measurement of one single *generalized* observable. By means of 'quantum tomography' state reconstruction can be achieved also in standard quantum mechanics; however, in general this method requires measurement of a large number of standard observables.

POVMs are obtained in a natural way when applying quantum mechanics to the interaction of object and measuring instrument. Thus, let $\rho^{(o)}$ and $\rho^{(a)}$ be the initial density operators of object and measuring instrument, respectively, and let $\rho^{(oa)}_{fin} = U\rho^{(o)} \otimes \rho^{(a)} U^\dagger$, $U = e^{-\frac{i}{\hbar}HT}$ be the final state of the interaction. If in this latter state a measurement is performed of the pointer observable $\{E^{(a)}_m\}$, then the measurement probabilities are found according to

$$p_m = Tr_{oa}\, \rho^{(oa)}_{fin} E^{(a)}_m = Tr_o \rho^{(o)} M_m, \tag{3}$$

with M_m given by

$$M_m = Tr_a \rho^{(a)} U^\dagger E^{(a)}_m U. \tag{4}$$

From expression (4) it follows that there is no reason to expect that M_m should be a projection operator; and in general it isn't.

The generalization of the mathematical formalism by means of the introduction of POVMs entails a considerable extension of the domain of application of quantum mechanics. In particular, it is possible that the set of operators $\{M_m\}$ of a POVM spans the whole of Hilbert-Schmidt space, in which case we have a *complete* measurement. Such *complete* measurements are experimentally feasible,[1–3] and may have considerable practical importance because of their richer informational content.

As can be seen from (3) and (4), it is the interaction of object and measuring instrument which is at the basis of the notion of a POVM. In quantum mechanics textbooks measurement is generally treated in an axiomatic way, and a detailed description of it is virtually absent. Bohr was one of the few to take the problem seriously, but he was mainly interested in the *macroscopic* phase of the measurement, which, according to him, was to be described by *classical* mechanics. However, not the macroscopic but rather the *microscopic* phase of the measurement, in which the microscopic information is transferred from the microscopic object to the measuring instrument, is crucial for obtaining *quantum* information. This phase should be described by quantum mechanics.

The influence of measurement has been of the utmost importance in the early days of quantum mechanics. In particular has it been a crucial feature at the inception of the notion of *complementarity*. In section 2 it will be shown that POVMs indeed play a crucial role there. By hindsight it can be concluded that much confusion could have been prevented if at that time it would have been realized that the standard formalism of quantum mechanics (as laid down, for instance, in von Neumann's authoritative book[4]) is just a preliminary step towards a more general formalism. As it is evident now, the standard formalism is not even able to yield a proper description of the so-called thought experiments, at that time being at the heart of our understanding of quantum mechanics.[2]

In this contribution the importance of the generalized formalism of POVMs is demonstrated by means of two examples, the first one elucidating Bohr's concept of complementarity in the sense of mutual disturbance of the measurement results of jointly measured incompatible standard observables (section 2). As a second example, in section 3 a *generalized* Aspect experiment is discussed using the POVM formalism, thus demonstrating that violation of the Bell inequalities can be seen as a consequence of complementarity rather than as being associated with nonlocality.

2. Complementarity

2.1. *The Summhammer, Rauch, Tuppinger experiment*

In this section I will now discuss as an example of the double-slit experiment a neutron interference experiment performed by Summhammer, Rauch and Tuppinger.[5] Other examples can be found in many different areas of experimental physics.[2] Let us first consider the two limiting cases which can be treated by means of standard

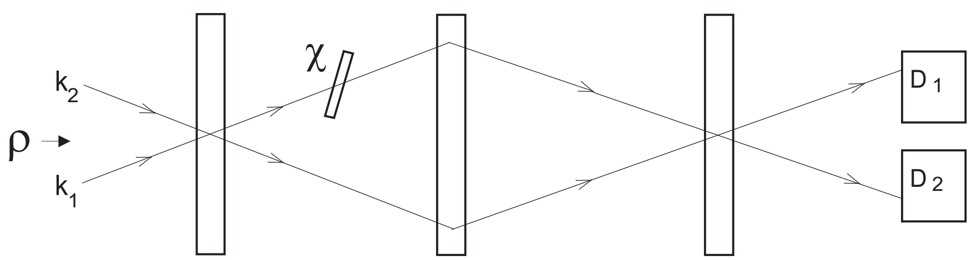

Fig. 1. Pure interference measurement.

quantum mechanics, viz. what I shall denote as the 'pure interference measurement' (cf. figure 1) and the 'pure path measurement' (cf. figure 2). In the figures a neutron interferometer is schematically represented by three vertical slabs in which Bragg reflection takes place and interference of the different paths can be realized after a possible phase shift χ has been applied in one of the paths. Detectors D_1 and D_2 can be placed either behind the third slab (figure 1), or behind the second one, in which case the experiment reduces to a 'which-path' measurement (in figure 2 this is realized by putting an ideal absorber in one path, while adding the measurement frequencies of detectors D_1 and D_2 to obtain the probability p_+ the neutron was in

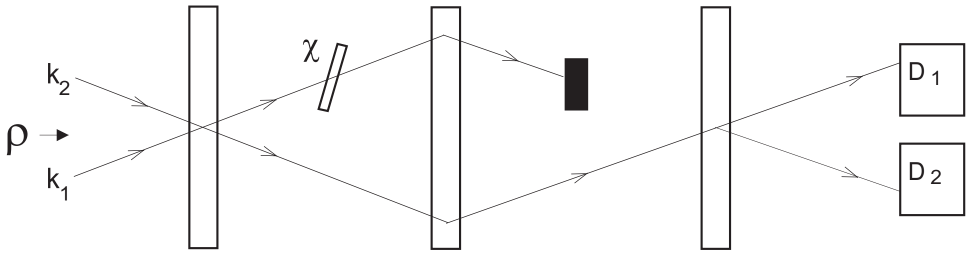

Fig. 2. Pure path measurement.

the second path; $p_- = 1 - p_+$ is the probability that the neutron was in the path of the ideal absorber).

The observables measured in the measurement arrangements of figures 1 and 2 are standard observables which can easily be found on the basis of elementary considerations.[6] With ρ the initial (incoming) state we find:
pure interference measurement: $p_n = Tr\rho Q_n,\ n = 1, 2,\ \{Q_1, Q_2\}$ the PVM of the standard interference observable;
pure path measurement: $p_m = Tr\rho P_m,\ m = +, -,\ \{P_+, P_-\}$ the PVM of the standard path observable.
It will not be necessary to display these observables explicitly; it is sufficient to know that the operators Q_n and P_m are projection operators, defining PVMs of standard quantum mechanics.

In the experiment performed by Summhammer, Rauch and Tuppinger[5] an absorber (transmissivity a) is inserted in one of the paths (figure 3). In the limits $a = 1$

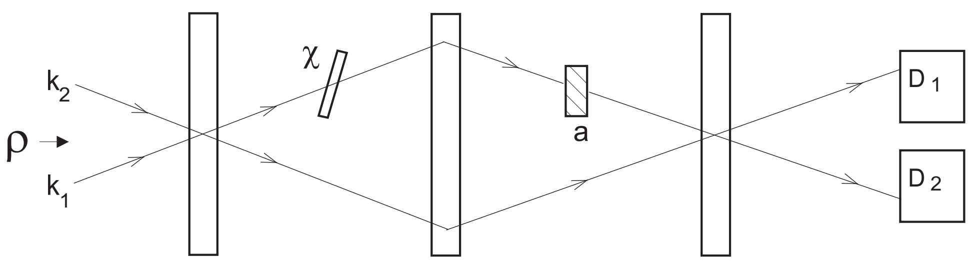

Fig. 3. Neutron interference measurement by Summhammer, Rauch and Tuppinger.

and $a = 0$ the Summhammer, Rauch, Tuppinger experiment reduces to the pure interference and the pure path measurement, respectively. The interesting point is that in between these limits the experiment is no longer described by a PVM, but by a POVM. Indeed, we find for $0 \leq a \leq 1$: $p_i = Tr\rho M_i, i = 1, 2, 3$, in which $i = 3$ refers to those events in which the neutron is absorbed by the absorber. It is easily seen[6] that the operators M_i are given according to

$$\begin{cases} M_1 = \frac{1}{2}[P_+ + aP_- + \sqrt{a}(Q_1 - Q_2)], \\ M_2 = \frac{1}{2}[P_+ + aP_- - \sqrt{a}(Q_1 - Q_2)], \\ M_3 = (1-a)P_-. \end{cases} \tag{5}$$

In the following way the measurement represented by the POVM $\{M_1, M_2, M_3\}$, M_i given by (5), can be interpreted as a joint nonideal measurement of the interference and path observables defined above. Define the bivariate POVM (R_{mn}) as follows:

$$(R_{mn}) := \begin{pmatrix} M_1 & M_2 \\ \frac{1}{2}M_3 & \frac{1}{2}M_3 \end{pmatrix}. \tag{6}$$

Then the two marginals, $\{\sum_m R_{mn}, n = 1, 2\}$ and $\{\sum_n R_{mn}, m = +, -\}$, are easily found. It directly follows from (5) that these marginals are related to the PVMs $\{Q_1, Q_2\}$ and $\{P_+, P_-\}$, respectively, according to

$$\begin{pmatrix} \sum_m R_{m1} \\ \sum_m R_{m2} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1+\sqrt{a} & 1-\sqrt{a} \\ 1-\sqrt{a} & 1+\sqrt{a} \end{pmatrix} \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix}, \tag{7}$$

$$\begin{pmatrix} \sum_n R_{+n} \\ \sum_n R_{-n} \end{pmatrix} = \begin{pmatrix} 1 & a \\ 0 & 1-a \end{pmatrix} \begin{pmatrix} P_+ \\ P_- \end{pmatrix}. \tag{8}$$

The important feature of (7) and (8) is that one marginal contains information only on the standard interference observable, whereas the other marginal only refers to the standard path observable. Actually, the bivariate POVM (6) was construed so as to realize this.

Equations (7) and (8) are applications of a general definition of a *nonideal* measurement,[7] to the effect that a POVM $\{M_i\}$ is said to represent a nonideal measurement of POVM $\{N_j\}$ if

$$M_i = \sum_j \lambda_{ij} N_j, \ \lambda_{ij} \geq 0, \ \sum_i \lambda_{ij} = 1.$$

This expression compares the measurement procedures of POVMs $\{M_i\}$ and $\{N_j\}$, to the effect that the first can be interpreted as a nonideal or inaccurate version of the second, the nonideality matrix (λ_{ij}) representing the nonideality. A convenient measure of this nonideality is the average row entropy of the nonideality matrix,

$$J_{(\lambda)} := -\frac{1}{N} \sum_{ij} \lambda_{ij} \ln \frac{\lambda_{ij}}{\sum_{j'} \lambda_{ij'}}, \ N \text{ the dimension of matrix } (\lambda_{ij}). \tag{9}$$

As is seen from (7) and (8) the measurement procedure depicted in figure 3 gives rise to two nonideality matrices, to be denoted by $(\lambda_{mm'})$ and $(\mu_{nn'})$, respectively. Under variation of the parameter a the nonideality matrices $(\lambda_{mm'})$ and $(\mu_{nn'})$ are seen to exhibit a behavior that is very reminiscent of the idea of complementarity as presented for the first time by Bohr in his Como lecture:[8] in one limit $(a = 1)$ ideal information is obtained on the standard interference observable, whereas no information at all is obtained on the standard path observable; in the other limit ($a = 0$) the roles of the standard interference and path observables are interchanged. For values $0 < a < 1$ we have intermediate situations in which information is obtained on the probability distributions of *both* standard observables, to the effect that information on one observable gets less accurate as the information on the other one gets more ideal. By changing the measurement arrangement so as to also obtain information on another (incompatible) standard observable, the information on the first observable gets blurred to a certain extent.

2.2. *The Martens inequality*

Complementary behavior as discussed above is a rather common feature of quantum mechanical measurement; many other examples can be given.[2] Using the nonideality measure $J_{(\lambda)}$ (9) it is possible to give a general account of this complementarity.[7] Let a bivariate POVM (R_{mn}) satisfy

$$\begin{array}{l} \sum_n R_{mn} = \sum_{m'} \lambda_{mm'} P_{m'},\ \lambda_{mm'} \geq 0,\ \sum_m \lambda_{mm'} = 1, \\ \sum_m R_{mn} = \sum_{n'} \mu_{nn'} Q_{n'},\ \mu_{nn'} \geq 0,\ \sum_n \mu_{nn'} = 1, \end{array} \tag{10}$$

in which $\{P_m\}$ and $\{Q_n\}$ are maximal PVMs. Then the corresponding nonideality

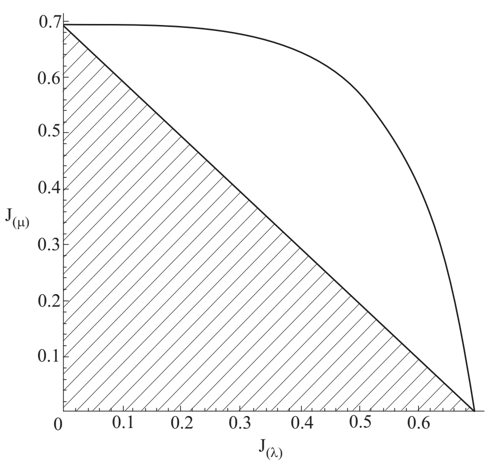

Fig. 4. Parametric plot of $J_{(\lambda)}$ and $J_{(\mu)}$ for the Summhammer, Rauch,Tuppinger experiment.

measures $J_{(\lambda)}$ and $J_{(\mu)}$ satisfy the *Martens inequality*[a]

$$J_{(\lambda)} + J_{(\mu)} \geq -\ln\{\max_{mn} Tr P_m Q_n\}.$$

[a]For nonmaximal PVMs this expression has to be slightly generalized.[7]

For the Summhammer, Rauch,Tuppinger experiment we obtain

$$J_{(\lambda)} = \frac{1}{2}[(1+a)\ln(1+a) - a\ln a],$$
$$J_{(\mu)} = \frac{1}{2}[2\ln 2 - (1+\sqrt{a})\ln(1+\sqrt{a}) - (1-\sqrt{a})\ln(1-\sqrt{a})].$$

In figure 4 a parametric plot is given of these quantities. The shaded area contains values of $J_{(\lambda)}$ and $J_{(\mu)}$ forbidden by the Martens inequality. This latter inequality, hence, does represent the Bohr-Heisenberg idea of complementarity in the sense of a mutual disturbance of the information obtained in a joint nonideal measurement of two standard observables.

2.3. *Martens inequality versus Heisenberg uncerainty relation*

It should be stressed that the Martens inequality is a general feature of quantum mechanical *measurement procedures* satisfying (10). In particular it is independent of the density operator ρ. This feature distinguishes the Martens inequality from the Heisenberg uncerainty relation

$$\Delta A \Delta B \geq \frac{1}{2}|Tr\rho[A,B]_-|, \tag{11}$$

A and B standard observables. It is interesting to remember that for a long time it has been the Heisenberg uncerainty relation (11) that was supposed to describe complementarity in the sense of mutual disturbance in a joint nonideal measurement of two standard observables. This has been questioned by Ballentine[9] to the effect that the Heisenberg inequalities (11) do not refer to *joint* measurement of incompatible observables at all, since they can be tested by *separate ideal* measurements of the two standard observables in question. According to Ballentine even "Quantum mechanics has nothing to say about joint measurement of incompatible observables."

As far as *standard* quantum mechanics is concerned, Ballentine is certainly right. However, as is seen from section 2.2, the *generalized* quantum mechanics of POVMs is able to deal with joint nonideal measurement of incompatible observables. The Martens inequality, rather than the Heisenberg inequality, is representing the concomitant complementarity. Although Bohr and Heisenberg had a perfect intuition as regards the physics going on in a double-slit experiment, they were not able to give a comprehensive treatment of it, due to the fact that they did not have at their disposal the generalized formalism of POVMs. As a consequence they were restricted to a discussion of the limiting cases only (in our example $a = 0$ and $a = 1$). They unjustifiedly thought[10] that the Heisenberg inequality (11) was the mathematical expression of their intuition on the intermediate cases (in our example corresponding to $0 < a < 1$). However, rather than the Heisenberg inequality it is the Martens inequality, derived from the generalized formalism, which serves this purpose. It seems that, due to a too one-sided preoccupation with measurement, Bohr and Heisenberg overlooked the possibility that not only *measurement* but also *preparation* might yield a contribution to complementarity, the Heisenberg uncertainty relations referring to the latter contribution.

3. Bell inequalities

As is well known, the Bell inequalities cannot be derived from *standard* quantum mechanics; they were derived by Bell[11] from a local hidden-variables theory. As a consequence, it is generally believed that violation of the Bell inequalities by the standard Aspect experiments[12,13] is a consequence of *nonlocality*. In this section it will be demonstrated that our understanding of the Bell inequalities, too, can considerably be enhanced by applying the generalized formalism.[2]

3.1. *Generalized Aspect experiment*

For this purpose the following experiment is considered, to be referred to as the *generalized Aspect experiment* (cf. figure 5). In the experiment each photon of a

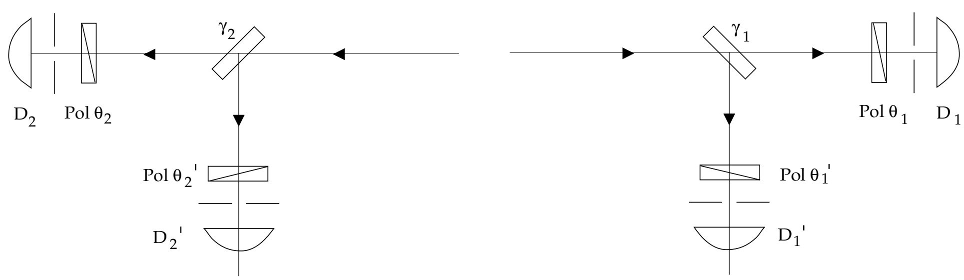

Fig. 5. Generalized Aspect experiment.

correlated photon pair impinges on a semi-transparent mirror (transmissivities γ_1 and γ_2, respectively). In the paths of the transmitted and reflected photon beams of photon i ($i = 1, 2$) polarization measurements are performed in directions θ_i and θ'_i, respectively. Using ideal detectors D_1, D'_1, D_2 and D'_2, a measurement result (occurrence or nonoccurrence of a click in each of the four detectors) is obtained for each individual photon pair. The four (standard) Aspect experiments[12,13] are special cases of the present experiment, satisfying $(\gamma_1, \gamma_2) = (1, 1)$, $(1, 0)$, $(0, 1)$ or $(0, 0)$, respectively (in each of these experiments the two detectors which are certain *not* to click have been omitted).

The generalized Aspect experiment can be analyzed, analogously to the discussion in section 2, in terms of complementarity in the sense of mutual disturbance in a joint nonideal measurement of incompatible standard observables. Let us first consider the measurement performed in one arm of the interferometer ($i = 1$ or 2). In agreement with definition (10) this measurement can be interpreted as a joint nonideal measurement of the (standard) polarization observables (PVMs) $\{E_+^{\theta_i}, E_-^{\theta_i}\}$ and $\{E_+^{\theta'_i}, E_-^{\theta'_i}\}$ in directions θ_i and θ'_i, respectively. Thus, by expressing, for a given i, the joint detection probabilities of photon detectors D_i and D'_i as $p_{m_i n_i} = Tr\rho R^{\gamma_i}_{m_i n_i}$, the bivariate POVM $(R^{\gamma_i}_{m_i n_i})$ is defined according to

$$(R^{\gamma_i}_{m_i n_i}) = \begin{pmatrix} O & \gamma_i E^{\theta_i}_+ \\ (1-\gamma_i)E^{\theta'_i}_+ & \gamma_i E^{\theta_i}_- + (1-\gamma_i)E^{\theta'_i}_- \end{pmatrix},\ i = 1,2. \tag{12}$$

The marginals of $(R^{\gamma_i}_{m_i n_i})$ are found as

$$\begin{pmatrix} \sum_{n_i} R^{\gamma_i}_{+n_i} \\ \sum_{n_i} R^{\gamma_i}_{-n_i} \end{pmatrix} = \begin{pmatrix} \gamma_i & 0 \\ 1-\gamma_i & 1 \end{pmatrix} \begin{pmatrix} E^{\theta_i}_+ \\ E^{\theta_i}_- \end{pmatrix} \text{ (detector D}_i\text{)}, \tag{13}$$

$$\begin{pmatrix} \sum_{m_i} R^{\gamma_i}_{m_i+} \\ \sum_{m_i} R^{\gamma_i}_{m_i-} \end{pmatrix} = \begin{pmatrix} 1-\gamma_i & 0 \\ \gamma_i & 1 \end{pmatrix} \begin{pmatrix} E^{\theta'_i}_+ \\ E^{\theta'_i}_- \end{pmatrix} \text{ (detector D}'_i\text{)}. \tag{14}$$

As functions of $\gamma_i,\ 0 \leq \gamma_i \leq 1$ the nonideality matrices in (13) and (14) show complementary behavior completely analogous to that of (7) and (8), and illustrated by figure 4. From this complementarity it can be concluded that, for instance, a measurement result for the polarization in direction θ_i, obtained in the generalized Aspect experiment ($0 < \gamma_i < 1$), can be different from one obtained if an *ideal* measurement of this standard observable ($\gamma_i = 1$) would have been performed. Moreover, it follows that this difference is a consequence of changing the measurement arrangement from $\gamma_i = 1$ to $\gamma_i < 1$, or vice versa. It is also seen that for $\gamma_i = 1$ the marginal (14) is given by $\{O, I\}$, which is a completely uninformative observable, not yielding any information on the state of photon i. This justifies the omission, referred to above, of the corresponding detector in the standard Aspect experiment.

The generalized Aspect experiment depicted in figure 5 can be interpreted in an analogous way as a joint nonideal measurement of the *four* standard observables $\{E^{\theta_1}_+, E^{\theta_1}_-\}$, $\{E^{\theta'_1}_+, E^{\theta'_1}_-\}$, $\{E^{\theta_2}_+, E^{\theta_2}_-\}$, and $\{E^{\theta'_2}_+, E^{\theta'_2}_-\}$, a quadrivariate POVM being obtained as the direct product of the bivariate POVMs given in (12):

$$R^{\gamma_1\gamma_2}_{m_1n_1m_2n_2} = R^{\gamma_1}_{m_1n_1} R^{\gamma_2}_{m_2n_2}. \tag{15}$$

From this expression it is evident that there is no disturbing influence on the marginals in one arm of the interferometer by changing the measurement arrangement in the other arm. Since observables referring to different objects do commute with each other, this is not unexpected. Complementarity in the sense of mutual disturbance of measurement results is effective in both of the arms *separately*, disturbance being caused in each arm by changing the measurement arrangement in that very arm.

3.2. *Complementarity and nonlocality as alternative explanations of violation of the Bell inequalities*

The interesting outcome of the present discussion of the generalized Aspect experiment is the existence of a *quadrivariate* probability distribution

$$p^{\gamma_1\gamma_2}_{m_1n_1m_2n_2} = Tr\rho R^{\gamma_1}_{m_1n_1} R^{\gamma_2}_{m_2n_2} \tag{16}$$

for the experimentally obtained measurement results. According to a theorem proven by Fine,[14] and by Rastall,[15] the existence of this quadrivariate probability distribution implies that the Bell inequalities are satisfied by the four bivariate marginals $p^{\gamma_1\gamma_2}_{m_1m_2}$, $p^{\gamma_1\gamma_2}_{m_1n_2}$, $p^{\gamma_1\gamma_2}_{n_1m_2}$ and $p^{\gamma_1\gamma_2}_{n_1n_2}$ which can be derived from (16) for fixed (γ_1, γ_2).

It should be noted that this holds true *also* for each of the *standard* Aspect experiments, corresponding to one of the limiting cases $(\gamma_1, \gamma_2) = (1, 1)$, etc.. Evidently, violation of the Bell inequalities by these experiments must be caused by the fact that no quadrivariate probability distribution exists from which the four bivariate probabilities $p^{\gamma_1=1\gamma_2=1}_{n_1n_2}$, $p^{\gamma_1=1\gamma_2=0}_{n_1m_2}$, $p^{\gamma_1=0\gamma_2=1}_{m_1n_2}$, and $p^{\gamma_1=0\gamma_2=0}_{m_1m_2}$ can be derived as marginals. So, the question to be answered is, why such a quadrivariate probability distribution does not exist, even though for each of the standard Aspect experiments separately one is given by (16).

A step towards answering this question is the observation that the quadrivariate probability distributions $p^{\gamma_1\gamma_2}_{m_1n_1m_2n_2}$ given by (16) are different for different (γ_1, γ_2): they depend on the measurement arrangement, and so, in general, do their marginals. Hence, changing the measurement arrangement from one standard Aspect experiment to another yields a disturbance of the measurement probabilities, preventing the Bell inequalities from being derivable from the existence of a single quadrivariate probability distribution.

In accepting this explanation we may choose between two different disturbing mechanisms, viz. nonlocality or complementarity. In the first case it is assumed that the probabilities in one arm of the interferometer are influenced in a nonlocal way by changing the measurement arrangement in the *other* arm. This is the explanation that is generally accepted. The alternative explanation, based on complementarity, takes into account the disturbing influence of a change of the measurement arrangement performed in an arm of the interferometer on the measurement probabilities measured in that *same* arm, as expressed by (13) and (14).

In deciding which of the alternatives, nonlocality or complementarity, to accept, it is important to realize that, if four standard observables (PVMs) $\{E^1_i\}$, $\{F^1_j\}$, $\{E^2_k\}$, and $\{F^2_\ell\}$ are mutually compatible, a quadrivariate probability distribution, viz. $Tr\rho E^1_i F^1_j E^2_k F^2_\ell$, exists even in the standard formalism. Hence, *in*compatibility is a necessary condition for violation of the Bell inequalities. But, since observables referring to causally disjoint regions of space-time do commute, only observables referring to the *same* region can be incompatible. Hence, *in*compatibility is a *local* affair, as, consequently, is violation of the Bell inequalities. It seems that complementarity can yield a *local* explanation of violation of the Bell inequalities, based on mutual disturbance in the joint nonideal measurements of incompatible standard observables carried out separately in each arm of the interferometer. Such an explanation could not be given on the basis of the standard formalism since, as demonstrated in section 2, that formalism is not able to deal with this kind of complementarity. Dependence on the measurement arrangement is only evident when considering the bivariate probabilities $Tr\rho R^{\gamma_i}_{m_in_i}$, derived from (12), which do not exist in the standard formalism.

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